



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:34 AM GMT

PDB ID : 2R8S  
Title : High resolution structure of a specific synthetic FAB bound to P4-P6 RNA ribozyme domain  
Authors : Ye, J.D.; Tereshko, V.; Sidhu, S.S.; Koide, S.; Kossiakoff, A.A.; Piccirilli, J.A.  
Deposited on : 2007-09-11  
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

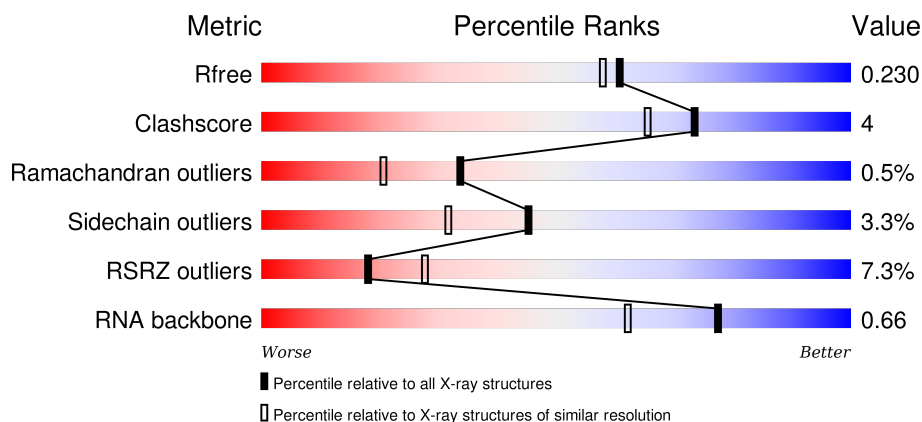
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)
RNA backbone	2183	1002 (2.70-1.24)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	R	159	<div> <div>9%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>
2	L	214	<div> <div>8%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
3	H	224	<div> <div>4%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	R	1001	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7217 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called P4-P6 RNA RIBOZYME DOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	159	Total	C	N	O	P	0	0	0
			3404	1522	623	1101	158			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	102	G	-	EXPRESSION TAG	GB 10840
R	103	G	-	EXPRESSION TAG	GB 10840
R	?	-	C	DELETION	GB 10840

- Molecule 2 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	4	0
			1644	1027	274	336	7			

- Molecule 3 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	219	Total	C	N	O	S	0	2	1
			1632	1031	271	321	9			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	R	4	Total	Mg	0	0
			4	4		

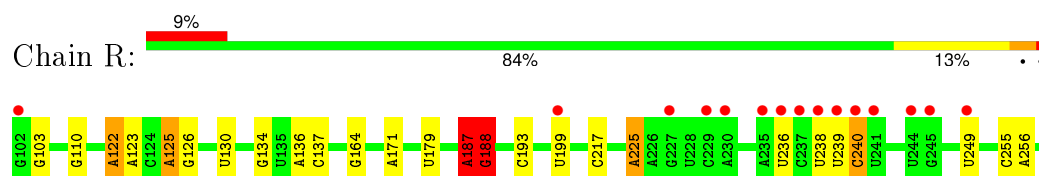
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	141	Total 141	O 141	0	0
5	L	131	Total 132	O 132	0	1
5	R	257	Total 260	O 260	0	3

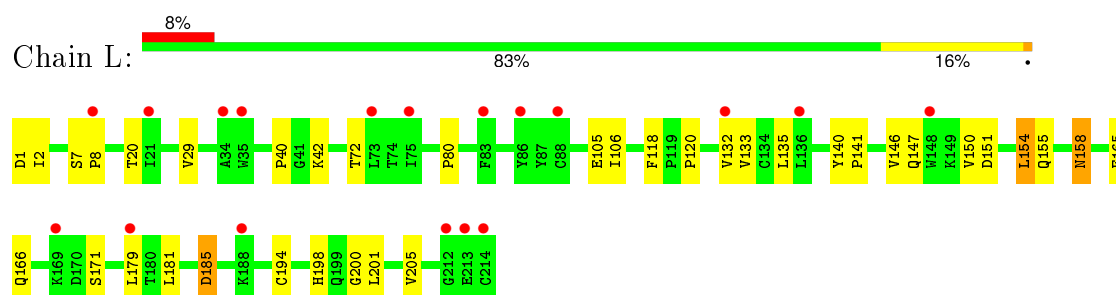
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

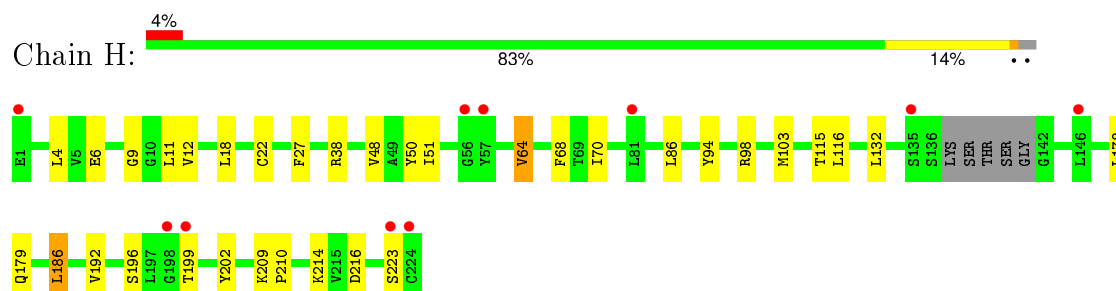
- Molecule 1: P4-P6 RNA RIBOZYME DOMAIN



- Molecule 2: Fab light chain



- Molecule 3: Fab heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.09Å 53.23Å 160.56Å 90.00° 108.42° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95 19.69 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.6 (20.00-1.95) 98.6 (19.69-1.95)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.195 , 0.226 0.199 , 0.230	Depositor DCC
$R_{free}$ test set	3875 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.0	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 58.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 77127 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7217	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	R	0.69	0/3812	1.21	12/5943 (0.2%)
2	L	0.45	0/1687	0.87	3/2288 (0.1%)
3	H	0.45	0/1682	0.84	0/2290
All	All	0.59	0/7181	1.07	15/10521 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	164	G	O4'-C1'-N9	9.15	115.52	108.20
1	R	193	C	O4'-C1'-N1	7.18	113.94	108.20
1	R	125	A	C1'-O4'-C4'	-6.33	104.83	109.90
2	L	151	ASP	CB-CG-OD2	6.17	123.86	118.30
1	R	134	G	N1-C6-O6	-6.08	116.25	119.90
1	R	122	A	P-O3'-C3'	5.97	126.86	119.70
1	R	171	A	O4'-C1'-N9	5.75	112.80	108.20
1	R	225	A	O4'-C1'-N9	5.55	112.64	108.20
1	R	240	C	C2-N1-C1'	5.52	124.88	118.80
1	R	110	G	N9-C1'-C2'	5.41	121.03	114.00
2	L	185	ASP	CB-CG-OD2	5.41	123.17	118.30
1	R	130	U	C3'-C2'-C1'	-5.34	97.22	101.50
1	R	188	G	O4'-C1'-N9	-5.29	103.97	108.20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1	ASP	CB-CG-OD2	5.29	123.06	118.30
1	R	187	A	C3'-C2'-C1'	5.03	105.52	101.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	7	SER	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	3404	0	1715	3	0
2	L	1644	0	1588	24	0
3	H	1632	0	1581	22	0
4	R	4	0	0	0	0
5	H	141	0	0	0	0
5	L	132	0	0	0	0
5	R	260	0	0	3	0
All	All	7217	0	4884	47	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (47) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:118:PHE:HB2	2:L:133:VAL:HG22	1.64	0.79
3:H:12:VAL:HG11	3:H:18:LEU:HG	1.69	0.72
3:H:4:LEU:HG	3:H:22:CYS:SG	2.32	0.69
2:L:198:HIS:CD2	2:L:200:GLY:H	2.16	0.64
2:L:118:PHE:HD2	2:L:133:VAL:HG23	1.62	0.64
2:L:147:GLN:OE1	2:L:154:LEU:HD11	1.99	0.62
5:R:1261:HOH:O	3:H:103[B]:MET:HE2	1.99	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:186:LEU:C	3:H:186:LEU:HD12	2.22	0.58
3:H:64:VAL:HG13	3:H:68:PHE:HB2	1.85	0.56
2:L:146:VAL:HG13	2:L:194[B]:CYS:SG	2.48	0.53
2:L:181:LEU:HD12	2:L:185:ASP:HB3	1.90	0.52
1:R:256:A:N7	5:R:1030[A]:HOH:O	2.34	0.51
3:H:178:LEU:HD13	3:H:179:GLN:O	2.11	0.50
3:H:9:GLY:H	3:H:115:THR:HG21	1.77	0.50
2:L:141:PRO:O	2:L:198:HIS:HE1	1.95	0.49
5:R:1261:HOH:O	3:H:103[B]:MET:CE	2.56	0.49
2:L:118:PHE:CD2	2:L:133:VAL:HG23	2.44	0.49
2:L:133:VAL:CG2	3:H:132:LEU:HD22	2.43	0.48
3:H:196:SER:HA	3:H:199:THR:HG22	1.96	0.47
2:L:133:VAL:HG21	3:H:132:LEU:HD22	1.96	0.47
2:L:2:ILE:HD13	2:L:29:VAL:HG12	1.96	0.46
2:L:20:THR:HG23	2:L:72:THR:CG2	2.46	0.45
2:L:120:PRO:HD3	2:L:132:VAL:HG22	1.97	0.45
2:L:155:GLN:HB3	2:L:158:ASN:HD21	1.81	0.45
3:H:12:VAL:HG21	3:H:86:LEU:HD13	1.98	0.45
3:H:51:ILE:HB	3:H:70:ILE:HG21	2.00	0.44
2:L:166:GLN:HG2	2:L:171:SER:HA	2.00	0.44
3:H:214:LYS:NZ	3:H:216:ASP:OD1	2.50	0.44
2:L:140:TYR:CG	2:L:141:PRO:HA	2.53	0.44
3:H:6:GLU:OE2	3:H:94:TYR:O	2.37	0.43
2:L:179:LEU:HG	2:L:181:LEU:HD23	2.01	0.43
2:L:150:VAL:HG22	2:L:155:GLN:NE2	2.34	0.43
3:H:12:VAL:HG13	3:H:18:LEU:HD21	2.01	0.42
2:L:158:ASN:H	2:L:158:ASN:HD22	1.67	0.42
3:H:38:ARG:HD3	3:H:48:VAL:HG11	2.02	0.42
1:R:187:A:H5'	1:R:188:G:OP2	2.20	0.42
3:H:12:VAL:HG21	3:H:86:LEU:CD1	2.50	0.41
3:H:209:LYS:N	3:H:210:PRO:CD	2.83	0.41
2:L:118:PHE:CD2	2:L:133:VAL:CG2	3.03	0.41
2:L:80:PRO:HA	2:L:106:ILE:HG13	2.01	0.41
1:R:136:A:H2'	1:R:137:C:O4'	2.20	0.41
3:H:4:LEU:HD13	3:H:27:PHE:HZ	1.86	0.41
2:L:140:TYR:CD2	2:L:141:PRO:HA	2.56	0.41
3:H:64:VAL:HG13	3:H:68:PHE:CG	2.55	0.41
2:L:201:LEU:HD22	2:L:205:VAL:CG2	2.51	0.41
3:H:192:VAL:HG11	3:H:202:TYR:CE1	2.56	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	214/214 (100%)	205 (96%)	8 (4%)	1 (0%)	34	21
3	H	217/224 (97%)	209 (96%)	7 (3%)	1 (0%)	34	21
All	All	431/438 (98%)	414 (96%)	15 (4%)	2 (0%)	34	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	8	PRO
3	H	223	SER

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	191/189 (101%)	185 (97%)	6 (3%)	47	34
3	H	181/184 (98%)	175 (97%)	6 (3%)	45	32
All	All	372/373 (100%)	360 (97%)	12 (3%)	45	33

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	42	LYS
2	L	105	GLU
2	L	135	LEU
2	L	154	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	L	158	ASN
2	L	165[A]	GLU
3	H	11	LEU
3	H	50	TYR
3	H	64	VAL
3	H	98	ARG
3	H	116	LEU
3	H	186	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	100	GLN
2	L	158	ASN
2	L	198	HIS
3	H	3	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	158/159 (99%)	14 (8%)	5 (3%)

All (14) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	103	G
1	R	123	A
1	R	125	A
1	R	126	G
1	R	179	U
1	R	187	A
1	R	188	G
1	R	199	U
1	R	217	C
1	R	236	U
1	R	238	U
1	R	239	U
1	R	249	U
1	R	255	C

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	122	A
1	R	125	A
1	R	188	G
1	R	225	A
1	R	240	C

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	R	159/159 (100%)	0.39	15 (9%)	11 17	30, 45, 96, 148	0
2	L	214/214 (100%)	0.61	18 (8%)	14 22	27, 38, 52, 78	2 (0%)
3	H	219/224 (97%)	0.45	10 (4%)	36 47	22, 36, 50, 75	1 (0%)
All	All	592/597 (99%)	0.49	43 (7%)	18 28	22, 38, 64, 148	3 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	224	CYS	11.4
2	L	214	CYS	10.4
2	L	213	GLU	9.3
1	R	238	U	8.7
3	H	223	SER	8.1
3	H	56	GLY	7.3
1	R	237	C	6.6
1	R	239	U	6.2
1	R	236	U	5.3
1	R	102	G	5.1
1	R	240	C	4.8
1	R	235	A	4.6
3	H	57	TYR	4.6
1	R	199	U	3.9
2	L	212	GLY	3.7
2	L	88	CYS	3.5
3	H	1	GLU	3.3
2	L	83[A]	PHE	3.2
2	L	21	ILE	2.9
2	L	132	VAL	2.9
2	L	35	TRP	2.9
3	H	146	LEU	2.8
2	L	75	ILE	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	L	148	TRP	2.7
3	H	198	GLY	2.6
2	L	179	LEU	2.6
3	H	135	SER	2.5
2	L	86	TYR	2.5
2	L	73	LEU	2.4
2	L	8	PRO	2.4
2	L	188	LYS	2.4
1	R	241	U	2.4
2	L	136	LEU	2.3
2	L	34	ALA	2.3
1	R	244	U	2.2
2	L	169	LYS	2.2
1	R	249	U	2.2
1	R	230	A	2.2
3	H	81	LEU	2.1
1	R	229	C	2.1
3	H	199	THR	2.1
1	R	227	G	2.1
1	R	245	G	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	R	1001	1/1	0.94	0.18	2.59	32,32,32,32	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	R	1002	1/1	0.94	0.16	1.97	36,36,36,36	0
4	MG	R	1004	1/1	0.89	0.09	-0.17	35,35,35,35	0
4	MG	R	1003	1/1	0.95	0.06	-2.83	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.